

Final

**FOCUS REPORT**  
**New Chemicals Program**

**PART I: BACKGROUND**

Written By: DHN

FOCUS DATE: 9/10/2007

FOCUS CHAIR: A. Binder

COMPANY: [REDACTED]

CASE NUMBER(S): P07-0639 through and

**PART II: SAT RESULTS**

HEALTH: 1-2 ECOTOX: 1 OCCUPATIONAL EXPOSURE: NR CONSUMER EXPOSURE: - ENVIRONMENTAL RELEASES: -

Additional SAT  
Information:

**PART III: OTHER FACTORS**

- a. PRODUCTION VOLUME: [REDACTED] kg/yr
- b. PROD VOL OTHER:
- c. USE: Gas hydration inhibitor
- d. REGULATORY HISTORY: NRC
- e. TEST DATA:
- f. IMPORTED ☒ MANUFACTURED ☐ BOTH ☐
- g. MSDS: ☒
- h. CATEGORY: CATEGORY 2:

**PART IV: SUMMARY OF SAT ASSESSMENT**

CASE NUMBER: P07-0639

FATE: [REDACTED], and

TOC = 60.2% (M)

liquid with mp < -30 C (M)

log Kow = 2.38 (HPLC), 0.53 (EPI)

S = 33 g/L at 20 °C or dispersible (P)

pH = 7.5 at 1% in water (M)

vp < 1.0E-6 mm Hg or torr at 25 °C (P)

bp = decomposition prior to boiling at 150 °C (M)

H < 1.0E-8 (P)

log Koc = 2.4 (P)

log fish BCF = 1.1 (P)

sorption to sludge = low

submitted test data for aerobic biodegradation were:

40% biodegradation in 28 d via DOC, thus, not readily biodegradable by the marine aerobic biodegradation test (OECD306)

-----  
time percent  
(d) (%)  
-----

7 0  
14 6  
21 25  
28 40  
60 20  
-----



not readily biodegradable  
less than 50% biodegradation in 60 d, thus, P2  
POTW removal = 0% based on no biodegradation in 7 d and low sorption  
time for complete ultimate aerobic biodegradation > months  
sorption to soils and sediments = low  
PBT Potential: P2B1T1

HEALTH: Absorption moderate all routes based on physical/chemical properties;

concern for delayed irritation to eyes based on data for [REDACTED];  
low to moderate concern for toxicity

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:

fish 96-h LC50 > 190.0 P  
fish (ZF) 96-h LC50 > 100.0 M S,N H64 pH7.5  
fish (ZF) 96-h NOEC EC0 = 100.0 M S,N H64 pH7.5  
daphnid 48-h LC50 > 130.0 P  
green algal 96-h EC50 c > 240.0 P  
SW algae 72-h EC50 c = 180.0 M S,N H24  
SW algae 72-h EC50 r = 180.0 M S,N H24  
fish chronic value > 40.0 P  
daphnid ChV > 30.0 P  
algal ChV c = 60.0 P  
SW algae ChV c = 130.0 M S,N H24  
SW algae ChV r = 130.0 M S,N H24

Predictions are based on SAR-nearest analog analysis using an [REDACTED]

[REDACTED] liquid with mp < -30  
C (M); log Kow = 2.38 (HPLC), 0.53 (EPI); S = 33 g/L at 20 °C or dispersible (P); pH7; effective  
concentrations based on 100% active ingredients and mean measured concentrations; hardness  
<150.0 mg/L as CaCO3; and TOC <2.0 mg/L;  
low concern for toxicity  
assessment factor = 10.0  
concern concentration = 1.0 mg/L (ppm)

## **PART V: RAD RISK RATIONALE: HUMAN HEALTH**

## **PART VI: SUMMARY OF EXPOSURE/RELEASE**

## **PART VII: FOCUS DECISION AND RATIONALE**

DISPOSITION: Drop

RATIONALE: P07-0639 was dropped from further review. Potential risks to human health were addressed by no inhalation expected. Concerns for potential risks to the environment were low based on low toxicity. This was a CEB D3 Drop.

## **PART VIII: CCD DISPOSITION / DD**

CCD:

# STRUCTURE ACTIVITY TEAM REPORT ver. 04/98

Case #: P-07-0639

DCN:

SAT Date: 8/31/2007

SAT Chair: V. Nabholz

Submitter:

Chemical Name:

CAS RN:

Trade Name:

Structure

Molecular Formula:

Molecular Wt.

WT%<500:

WT%<1000:

MP:

BP:

dec. >150

Eq. Wt:

H2O Sol (g/L):

32.9

V.P.

<0.000001

Max. Prod. Volume (kg/yr):

Physical State:

Liquid

USE:

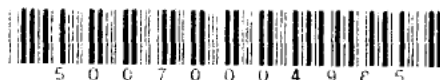
Gas hydration inhibitor.

Related Case Numbers	Case Role	Related Case Numbers	Case Role

Focus Date: SEP 10 2007

Results:

*DROP*  
Page 1 of 5



CASE NUMBER: P07-0639

RELATED CASES:

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN: HEALTH ECOTOX

LEVEL: 1-2 1

KEYWORDS: LUNG, IRR-E

SUMMARY OF ASSESSMENT:

FATE: [REDACTED], and

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POTW removal = 0% based on no biodegradation in 7 d and low  
sorption

time for complete ultimate aerobic biodegradation > months

sorption to soils and sediments = low

PBT Potential: P2B1T1

\*CEB FATE: migration to ground water = rapid

HEALTH: Absorption moderate all routes based on  
physical/chemical properties;

concern for delayed irritation to eyes based on data for [REDACTED]

low to moderate concern for toxicity

\*CEB HEALTH: Exposures to humans: inhalation

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:

fish 96-h LC50	>	190.0	P
fish (ZF) 96-h LC50	>	100.0	M S,N H64 pH7.5
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with and ; liquid with mp < -30 °C (M); log Kow = 2.38 (HPLC), 0.53 (EPI); S = 33 g/L at 20 °C or dispersible (P); pH7; effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150.0 mg/L as CaCO3; and TOC <2.0 mg/L;

low concern for toxicity

assessment factor = 10.0

concern concentration = 1.0 mg/L (ppm)

\*CEB ECOTOX: No releases to water

SAT Co-chair: Vince Nabholz, 564.8909

## NCSAB SAT REPORT

PMN: P-07-0639

CAS RN:

Chemical Name:

Analog:

Production Volume:

Structure:

Use:

Gas hydration inhibitor.

Formula:

Eq Wt:

Mol Weight:

Wt%&lt;500:

Wt%&lt;1000

MP:

BP:

dec. &gt;150

VP:

&lt;0.000001

H<sub>2</sub>O Sol (g/L):

32.9

Physical State:

Liquid

Log P:

Endpoint (mg/L)

Est. Value

Meas. Value

Comments

EOS

Fish 96-h

&gt; 1.9

Daphnid 48-h

&gt; 1.3

Algal 96-h

&gt; 2.4

Fish ChV

&gt; 0.38

Daphnid ChV

&gt; 0.26

Algal ChV

&gt; 1.2

BCF

CHEMICAL CLASS:

SAR:

ECOTOX CONCERN

H

(M)

L

CONCERN CONCENTRATION

0.026

DATE

8/31/07

ASSESSOR:

## ATTENDEES

## SIGNATURE

## CHEMISTRY

☐ Paul Bickart  
☐ Diana Darling  
☐ Rich Engler  
☐ Greg Fritz  
☐ Daniel Lin  
☒ Kathy Schechter

*Kathy Schechter*

## ENVIRONMENTAL FATE

☐ Bob Boethling  
☐ Wen-Hsiung Lee  
☐ Laurence Libelo  
☒ David Lynch  
☐ Andy Mamantov

MEMO

## HEALTH

☒ Katherine Anitole  
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☐ Steve Cragg  
☒ Leonard Keifer  
☒ David Lai  
☒ Jim Murphy  
☐ Deborah Norris  
☒ Ronald Ward  
☐ Yin Tak Woo

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*Michael Cimino*

*Leonard Keifer*  
*David Lai*

MEMO

MEMO

## ENVIRONMENTAL EFFECTS

☒ Gordon Cash  
☐ Vince Nabholz  
☐ Maggie Wilson

MEMO

## SAT CHAIR/OTHER

☐ Rebecca Jones  
☒ Leonard Keifer  
☒ Vince Nabholz  
☐ Jim Kwiat

*Leonard Keifer*